Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 310 (2016) 33–57
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Resolvent sampling based Rayleigh–Ritz method for large-scale nonlinear eigenvalue problems

Jinyou Xiao[a], Shuangshuang Meng[a], Chuanzeng Zhang[b,*], Changjun Zheng[c]

[a] School of Astronautics, Northwestern Polytechnical University, Xi'an 710072, China
[b] Department of Civil Engineering, University of Siegen, D-57068 Siegen, Germany
[c] Institute of Sound and Vibration Research, Hefei University of Technology, Hefei, 230009, China

Received 20 November 2015; received in revised form 11 May 2016; accepted 14 June 2016
Available online 28 June 2016

Abstract

A new algorithm, denoted by RSRR, is presented for solving large-scale nonlinear eigenvalue problems (NEPs) with a focus on improving the robustness and reliability of the solution, which is a challenging task in computational science and engineering. The proposed algorithm utilizes the Rayleigh–Ritz procedure to compute all eigenvalues and the corresponding eigenvectors lying within a given contour in the complex plane. The main novelties are the following. First and foremost, the approximate eigenspace is constructed by using the values of the resolvent at a series of sampling points on the contour, which effectively circumvents the unreliability of previous schemes that using high-order contour moments of the resolvent. Secondly, an improved Sakurai–Sugiura algorithm is proposed to solve the projected NEPs with enhancements on reliability and accuracy. The user-defined probing matrix in the original algorithm is avoided and the number of eigenvalues is determined automatically by the provided strategies. Finally, by approximating the projected matrices with the Chebyshev interpolation technique, RSRR is further extended to solve NEPs in the boundary element method, which is typically difficult due to the densely populated matrices and high computational costs. The good performance of RSRR is demonstrated by a variety of benchmark examples and large-scale practical applications, with the degrees of freedom ranging from several hundred up to around one million. The algorithm is suitable for parallelization and easy to implement in conjunction with other programs and software.

Keywords: Nonlinear eigenvalue problems; Rayleigh–Ritz procedure; Finite element method; Boundary element method

1. Introduction

The natural frequency λ and natural mode v are important parameters in the design of engineering structures and systems. Mathematically, they are the eigenvalue and the corresponding eigenvector satisfying the eigen-equation

$$T(\lambda)v = 0, \tag{1}$$

* Corresponding author.
E-mail addresses: xiaojy@nwpu.edu.cn (J. Xiao), c.zhang@uni-siegen.de (C. Zhang), cjzheng@hfut.edu.cn (C. Zheng).

http://dx.doi.org/10.1016/j.cma.2016.06.018
0045-7825/

where $T(z) \in \mathbb{C}^{n\times n}$ is a matrix-valued function depending on a parameter $z \in \mathcal{D} \subset \mathbb{C}$. When the matrix $T(z)$ in terms of z is nonlinear, equation (1) becomes the so-called nonlinear eigenvalue problem (NEP). Except for the quadratic eigenvalue problem that has been well-studied in the dynamic analysis of structures [1], the numerical solution of general NEPs still remains a challenging task, especially at large scales [2–4].

This work is concerned with developing efficient numerical methods for large-scale NEPs. In particular, we consider NEPs in the *finite element method* (FEM) and the *boundary element method* (BEM), since these two methods are extensively applied in computational science and engineering, either independently or in coupled manners [5,6]. Their NEPs reflect the main bottlenecks in the current development of numerical methods for NEPs. In the FEM, NEPs are often caused by the z-dependent material properties and/or boundary conditions, examples including the analysis of structures involving viscoelastic materials [7–9], free vibration of plates and shells with elastically attached masses [10], vibrations of fluid–solid structures [11], special treatment of artificial boundary conditions [12], etc. Typically, the FEM matrix $T(z)$ is sparse, symmetric, real and positive or semi-positive definite. These properties greatly benefit the numerical treatment. However, the situations in the BEM are totally different. The eigenvalue problems are in general strongly nonlinear even if the underlying physical problem is linear [13–15]. The matrix $T(z)$ is typically complex, dense and unstructured, making the evaluation of $T(z)$ itself and the operations with $T(z)$ (e.g., applying to vectors, solving linear systems, etc.) computationally very expensive. Besides, the entries of $T(z)$ are usually distinct functions of z whose dependence on z can hardly be expressed in explicit forms. All these factors contribute to the immense difficulties of solving the NEPs in BEM even with the state-of-the-art techniques [16,17]. Similar difficulties also exist in the NEPs in the coupled FEM-BEM [18,6].

In order to overcome the aforementioned difficulties in large-scale engineering applications, this paper aims at developing an eigensolver that simultaneously satisfies the following two requirements:

R1: it can robustly and reliably compute all the eigenvalues (and the corresponding eigenvectors) in a given region of the complex plane.

R2: it can solve large-scale NEPs (e.g., degrees of freedom (DOFs) n up to several millions) no matter the matrix $T(z)$ is dense or sparse, structured or unstructured, and allow for an easy implementation and efficient parallelization.

We notice that although there exist a number of algorithms for the solution of NEPs (see e.g., [19–23,17]), most of them are excluded by the above two requirements.

Essentially, existing numerical approaches for NEPs fall into three categories [19,24]. The first and classical approach is to formulate the NEP as a system of nonlinear equations and to use different variants of Newton's methods. Examples include the residual inverse iteration method [25], the Jacobi–Davidson method [26,21] and the block Newton method [22]. Typically, Newton type methods are only locally convergent and need good initial guess of the eigenvalues. The Jacobi–Davidson method can be used to determine several eigenvalues subsequently, but special strategies are required to avoid the repeated convergence towards the same eigenvalues [21,22]. Recently, a deflation strategy based on the concept of minimal invariant pairs has been proposed and integrated into the Jacobi–Davidson method for the robust and successive computation of several eigenpairs [17]. However, one should notice that, in all these methods, the repeated solution of the *correction equation* during the iterative process can be computationally very expensive for large-scale problems. Newton type methods applied to small BEM eigenvalue problems can be found in, e.g., [27].

The second approach transforms the NEP into a linear eigenvalue problem which can be solved by existing linear eigensolvers. This is a standard technique in solving quadratic eigenvalue problems in the FEM [1]. The applications to the NEPs in the BEM can be found in [14]. Recently, linearization by the polynomial or rational approximation of $T(z)$ has attracted increasing attention in solving medium and large NEPs; see, e.g., [16,24,28,29]. In particular, the compact rational Krylov method in [30] exploits the structure of the linearization pencils by using a generalization of the compact Arnoldi decomposition. As a result, the extra memory and orthogonalization costs are negligible for large-scale problems. Whereas, for the linearization-based methods there is still a need to construct linearizations that reflect the structure of the given matrix polynomial and to improve the stability of the linearizations [1,31]. Moreover, this class of methods is not suitable for large-scale BEM applications, because the storage of all the $n \times n$ coefficient matrices of $T(z)$ in a polynomial basis, even in compressed forms [32], would require huge memory.

The third approach, called *contour integral method*, is based on the contour integral of the resolvent $T(z)^{-1}$ applied to a full-rank matrix $U \in \mathbb{C}^{n\times L}$. This approach is first developed for solving generalized eigenvalue problems [33,34], and later, extended to solving NEPs in [35] and [23], respectively, using the Smith form and Keldysh's theorem